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SHARP Structural Mechanics Verification & Validation Plan

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1 Introduction

The objective of the NEAMS ToolKit is to develop a "pellet-to-plant" simulation capability useful for predicting performance and safety for a broad range of nuclear reactor power systems. Development of the ToolKit is being undertaken in support of the ongoing R&D programs in the U.S. Department of Energy (DOE) Office of Nuclear Energy (DOE-NE), as outlined in the Nuclear Energy R&D Roadmap. The NEAMS ToolKit is organized under a Fuels Product Line (FPL), a Reactors Product Line (RPL) and Integration Product Line (IPL) to be modular in design. The modeling approach and system integration architecture reflects the need to simulate a broad range of nuclear reactor power systems. Within the RPL, the reactor simulation functionality is provided by SHARP (Simulation-based High-efficiency Advanced Reactor Prototyping). SHARP comprises codes for neutronics , thermal-fluids and structural mechanics, that exchange information during coupled simulations via a common data infrastructure.

The NEAMS structural modules provides structural mechanics and material performance analysis. The structural mechanics module, based on the Diablo code (Solberg, et al., 2014), supports continuum-scale analysis of structural performance of integrated structures, such as fuel assemblies, reactor vessels, and containment buildings. Diablo provides an implicit finite-element simulation capability for nonlinear solid mechanics on large-scale parallel computers. It also has capabilities for conduction heat transfer, and as the SHARP team's experience with multi-physics reactor simulation builds, it may be found useful to have the Nek5000 (thermal hydraulics) and Diablo codes partition or otherwise share the duties of solving for updates to the reactor temperature field. An initial structural mechanics capability will be available as part of the FY2015 early user version, and a fully enabled version will be part of the FY2018 release.

The RPL encompasses broad simulation functionalities. To date, the primary focus of SHARP development has been the analysis of sodium fast reactor (SFR) configurations, e.g., ABTR (Merzari, et al., 2014). The performance of such fast-spectrum reactors is sensitive to structural deformations. It is therefore appropriate that this first V&V plan for structural mechanics be centered on structural response behaviors important to that class of problems. This plan is focused upon structural mechanics: multi-physics modeling of fast reactors is rightly the topic of a collective SHARP V&V plan. Likewise, expansion of structural mechanics into other application areas, e.g., seismic response analysis, would be supported by additional V&V plans.

2 Acronyms

Acronym	Definition
ABTR	Advanced Burner Test Reactor
ANL	Argonne National Laboratory
ASC	NNSA's Advanced Simulation & Computing
ASME	American Society of Mechanical Engineers
EBR-II	Experimental Breeder Reactor - II
FFTF	Fast Flux Test Facility
LLNL	Lawrence Livermore National Laboratory
MDG	Methods Development Group, LLNL
NAFEMS	A not-for-profit limited company focused on quality practices in engineering analysis, initially formed in 1983 as the National Agency for Finite Element Methods and Standards at the UK's National Engineering Laboratory. http://www.nafems.org/
NEAMS	Nuclear Energy Advanced Modeling & Simulation
NEUP	Nuclear Energy University Partnership
NNSA	DOE's National Nuclear Security Agency
SHARP	Simulation-based High-efficiency Advanced Reactor Prototyping
UQ	Uncertainty Quantification
V&V	Verification and Validation

3 Description of the Computational Model to be Validated

Diablo is an engineering multi-physics simulation code designed for scalable performance on parallel computer architectures with a primary focus on implicit analysis. Each “physics” is defined as a distinct discipline of engineering science, such as solid mechanics, heat transfer, or electromagnetics, in which the spatial and temporal variations of specified field quantities (e.g., displacements, rotations, temperatures) are governed by physical conservation laws. In the context of the NEAMS Toolkit, we are focused upon the structural and solid mechanics capabilities of Diablo.

Diablo grows out of the long history of successful engineering codes for solving single physics problems produced by the Methods Development Group (MDG) at LLNL, such as the explicit solid mechanics code DYNA3D, the implicit solid mechanics code NIKE3D (Puso, 2012), the thermal mechanics code TOPAZ3D, and the parallel explicit solid mechanics code ParaDyn. The strategy with Diablo has been to incorporate multiple field theories from the outset as MDG’s considerable implicit finite element capabilities are migrated to contemporary, large-scale parallel platforms.

3.1 Phenomena identification (e.g., PIRT); specific conditions, behavior, events the computational model must be able to predict/simulate.

A Phenomena Identification and Ranking Table (PIRT) can be a means for stakeholders to collectively denote and prioritize the physical behaviors that must be resolved (Technical Program Group, 1990) to have adequate understanding of some system. In the computational setting this concept has been adopted to a Predictive Capability Maturity Model (Oberkampf, Pilch, & Trucano, 2007). Given that the Diablo team has limited Nuclear Energy application experience, we believe it will be useful to start with a PIRT to focus on the physical behaviors relevant to future nuclear engineering users. Engagement with early adopters will thus be critical and serve a useful education function for the structural mechanics developers.

3.2 Description of the physics and empirical models embodied in the computational model, type and degree of physics coupling,

Diablo is a general purpose, implicit, nonlinear thermo-mechanics code suitable for simulation of relatively slow, or steady-state, phenomenon. Spatial discretization is focused on hexahedral continuum, quadrilateral structural shells and two-node beams. Material stress response models include elasticity (isotropic, orthotropic), plasticity, soil (Ramberg-Osgood), crushable and hyperelastic foams. Material thermal response models include conduction (isotropic, orthotropic), phase change, and enclosure grey-body radiation. A few material models specific to nuclear reactor materials have been included from the MATPRO library made available to the public by the Nuclear Regulatory Commission (Siefken, 2001).

The code uses Lagrangian finite elements with second order time and spatial convergence. For solid mechanics, time integration is focused on the Newmark method, which provides (linear) unconditional temporal stability while requiring the repeated solution of coupled linear systems of equations. For thermal mechanics, time integration is focused on the generalized-alpha method, which also provides unconditional temporal stability (in the linear case) while requiring the solution of coupled systems of equations. Both parallel direct and iterative linear solver options are available. Multiple field equations are solved through an operator splitting construct that repeatedly loops over the active sub-problems within each time step until the sub-problems simultaneously converge, optionally embedded within a global Quasi-Newton strategy. Multiple strategies are available to drive the nonlinear solution process for each of the field problems. The code provides an eigensolver used to identify free modes of structural vibration. This feature can be useful for verification of model inputs.

A unique feature of Diablo is its incorporation of a methodology for nonlinear soil-structure interaction (SSI) in the setting of time-domain integration. This work represents a generalization of a frequency domain method (Bielak, Loukakis, Hisada, & Yoshimura, 2003), which has been the traditional setting for SSI. However, seismic response is not an immediate priority of the Reactor Product Line, and this Plan will not incorporate any further discussion of that problem class.

3.3 Toolkit elements needed, libraries used, etc.

Diablo leverages a number of third-party libraries:

ARPACK	– Eigensolver package
EXODUSSII	– Mesh data description
FEMSTER	– Electromagnetics element formulation
HYPRE	– Iterative linear equation solvers
HDF5	– Data file format and access utilities
MILI	– Native visualization output format for Diablo
METIS	– Graph partition library for domain decomposition
MUMPS	– Direct linear equation solver
OVERLINK	– Mesh transfer utility
PWSSMP	– Direct linear equation solver
SILO	– Native visualization file format for Visit

When operating within SHARP, Diablo also directly uses these additional third-party libraries:

MOAB/ITAPS	– Mesh data storage utilities
NETCDF	– Data file format and access utilities
PARMETIS	– Graph partition library for domain decomposition
ZOLTAN	– Mesh decomposition and remapping utilities

When operating within the broader RPL, Diablo will interact with the MOOSE framework, but it is currently intended that data pipeline will be supplied through extensions to the MOAB.

3.4 Consequence of failure, risk grading, QRL

The NEAMS Verification and validation Plan Requirements document (Versluis, 2013) defines three Quality Rigor Levels. As the Structural Mechanics has been evolving through successive stages of integration with SHARP via MOAB it has been appropriate to assign it to QRL 3, "…generally applied to research and development activities that are exploratory, preliminary or investigative in nature." During this phase, our development efforts have benefited from the ongoing SQA practices at LLNL such as regression testing, issue tracking and technical reviews. As the full SHARP integration is realized and early adopters continue to exercise our capabilities, it will be appropriate to escalate to QRL 2 to support "activities such as viability R&D and performance R&D of advanced reactor concepts." Producing this V&V Plan is a first step in that process. Engagement with expert early-adopters will help drive the subsequent specification, construction and documentation of benchmark validation studies.

3.5 Hardware and software platforms. Software architecture, platform, data backplane, problem setup, results analysis and visualization. Discuss how hardware and software platforms influence validation.

The Diablo code is developed for execution on high-performance clusters that feature a high-bandwidth, low-latency interconnect. Such systems remain the purview of Unix/Linux operating systems. The code utilizes an object-based, hierarchic data model to represent the finite element problem in Fortran 95/2003 data structures. Algorithmic procedure functions advance the solution process, traversing through the data model. The code links to a number of C/C++ libraries and is itself 'capped' by a C main function to facilitate be accessed by other drivers such as SHARP's CouPÉ utility.

Diablo does not itself contain any 'set-up' utilities. LLNL analysts typically utilize TrueGrid or Cubit for mesh generation. The former provides ASCII text for mesh input, while for the latter Diablo can read from an EXODUSII-format file. The NiCE environment funding through the Integration Product Line will eventually provide a NEAMS Toolkit specific perspective and user portal.

Hardware and software will not have a major impact on these validation studies. Most target problems will be steady or quasi-steady where high-frequency response is not of physical interest. This translates to minimal impact due to order-of-operations in finite precision arithmetic. This does not mean that results will be invariant with respect to a) compiler optimization levels, b) choice of number of partitions for parallel processing, of c) hardware processor type. Nevertheless, these variations should be small and easily assessed through engineering judgment. If a case is found where such variations are at a troubling magnitude, then they will be investigated as either a manifestation of a code defect or the specific validation problem having behaviors such as bifurcation that are inherently susceptible to small variations. If the latter case, the problem must either be reformulated or acceptance criteria identified which reflect this physical variability.

4 Model Verification and Validation

We will be heavily influenced by the perspectives and terminology of the ASME Standards Committee on Verification and Validation in Computational Solid Mechanics (ASME, 2006), (ASME, 2012). The author has been a voting member of that committee for the past seven years, adding his code development perspectives to their deliberations.

4.1 Verification: Configuration management, version control. Problem reporting, corrective action, documentation. Static analysis

The software QA practices of the Diablo team are first governed by LLNL policy (LLNL, 2014a). This policy distinguishes between in-house developed and procured software tools. Software that performs a safety function related to 10 CFR 835, Occupational Radiation Protection, in a nuclear or radiological facility is referred to as “830 Software”. Diablo has not been assigned to that latter category. All software is required to undergo a risk grading (LLNL, 2014b), which then correlates to a set of required SQA practices. The Advanced Simulation & Computing program at LLNL has further policy (Pope, 2012), defining minimum practices to be met even if not required by the institutional policy.

One source of solid and structural mechanics verification problem definitions, and target solutions, are the NAFEMS benchmarks. Some of these have been successfully exercised with Diablo, e.g., (Ferencz & Greer, 2003). Others problems come from the academic literature or community (Wenk, 2007). Unfortunately, as finite deformation kinematics intersect with nonlinear material models, analytical solutions become scarce, and many verification problems will rely upon solutions by other finite element codes or via alternative numerical methodologies.

4.2 Applicable benchmarks and experimental data collections for validation

The immediate focus of our validation efforts will be to establish the basis for confidence in the structural mechanics module as a single-physics simulation tool. This will be foundational to validating SHARP in its intended multi-physics context. Unfortunately, data for structural mechanics response in fast reactor applications appears to be mostly available from legacy integral experiments, e.g., (Hecht & Trenchard, 1990), (Wigeland, 1987). More recent PHENIX experiments could be another target (Fontaine, et al., 2011), although sufficiently detailed disclosure in an international setting may be a challenge. The availability of any targeted structural mechanics single-effects tests would be welcome news. Absent any existing controlled, single-effects experimental data, one could envision its eventual development through a scaled experiment looking at a single duct-grid joint and then a three-duct grouping. These could be placed under mechanical loads and/or differentially heated to induce lateral deformations.

4.2.1 Unit, component, subsystem, system, integral tests, etc.

In software engineering, 'unit testing' is usually associated with test drivers for individual functions/subroutines/modules. Due to the voluminous data structures associated with finite element meshes, we do not feel it is productive to resort to testing at this fine granularity. Essentially one would replicate much of the balance-of-code to provide the data needed to drive the tested unit. We prefer to concentrate on well-posed solid and structural mechanics problems, with variations to test alternative functionality systems, e.g., contrasting element formulations or linear solvers. Quite often a simple mesh geometry will be replicated multiple times to then test different material models over different load or displacement histories. These may be broadly viewed as integral tests of the code, but with targeted goals for particular functionality tests.

4.2.2 Validation gaps

To date, no validation studies for nuclear power applications have been undertaken for Diablo.

4.2.3 Validation matrix

A key structural mechanics concern for fast reactors is the deformation of the fuel assembly ducts, typically hexagonal in cross section. Thermally driven deformation will influence neutronics performance and are fundamental to notions of passive safety. Long-term creep and swelling under normal operating conditions may lead to permanent distortions that impact serviceability such as the extraction of ducts for re-fueling activities. Our initial validation matrix, Table 1, thus focuses on a progression of problems that will provide confidence in the predictions of thermally-driven distortions and material response. Initial comparison will be against other analytical studies, e.g., (Grudzinski & Grandy, 2014), so that we can assure equivalence of boundary conditions. For example, one open issue is the appropriate representation of the duct and its 'socket' in the grid spacer. Understanding this in an analytical setting, before considering the variability of physical assemblages, will be worthwhile. It will also enable progress while identification of well-documented physical experiments, past and hopefully future, are identified.

Table 1. Validation progression for assessing NEAMS structural mechanics single-physics modeling

Phenomena	Validation Test	Data Source	Description
Inelastic creep at elevated temperature material response	Uniaxial and multi-axial loading configurations	MATPRO legacy model forms plus material-specific parameterizations	Verify quadrature-point implementation of baseline creep model, exercise in test coupon geometries, and compare with target material response.
Irradiation swelling material response	Uniaxial and multi-axial loading configurations	MATPRO legacy model forms plus material-specific parameterizations	Verify quadrature-point implementation of baseline swelling model, exercise in test coupon geometries, and compare with target material response.
Single duct warpage due to creep	Inelastic bending response under time-evolved temperature gradient(s)	(Grudzinski & Grandy, 2014)	Compare inelastic response under kinematic BCs of a limited bow core restraint system and assure proper qualitative behavior illustrated in report.
Single duct warpage due to swelling	Inelastic bending response under time-evolved fluence/dose	(Grudzinski & Grandy, 2014)	Compare inelastic response under kinematic BCs of a limited bow core restraint system and assure proper qualitative behavior illustrated in report.
Single duct warpage due to combined creep and swelling	Inelastic bending response under time-evolved fluence/dose	(Grudzinski & Grandy, 2014)	Compare inelastic response under kinematic BCs of a limited bow core restraint system and assure proper qualitative behavior illustrated in report.

Multi-duct contact due to warpage	Inelastic bending response under time-evolved temperature and fluence/dose	This may be more a functionality demonstration building toward subsequent entry	Compare contact behavior and pad-to-pad forces during response under kinematic BCs of a limited bow core restraint system
Core-sector duct ensemble response	Inelastic bending response under time-evolved temperature and fluence/dose	(Hecht & Trenchard, 1990)	Compare contact behavior and pad-to-pad forces during response under kinematic BCs of a limited bow core restraint system

4.2.4 Schedule, priorities

As illustrated, our priorities will first focus on establishing a pedigree for the structural mechanics capabilities most central to fast reactor modeling. Refinement of this plan after stakeholder comment will then lead to launching initial efforts in FY15.

5 Uncertainty quantification (UQ)

As per ASME recommended practice for computational solid mechanics, some level of UQ should be incorporated into validation studies. This can have multiple manifestations, including sensitivity analysis to explore the sources of variability in computational results—or the physics itself, formal propagation of uncertainties through the computational model, or perhaps as an entry point, simple elicitation of expert opinion. Experimental variability is likely to be best characterized for smaller, more focused experiments, e.g., material coupon tests. Replicates of expensive integral tests are often a good intention overtaken by fiscal realities.

Early efforts with UQ will examine the influence of parameters for which detailed physical characterization are likely lacking. For instance, using Dakota, explore the impact of pad-to-pad friction on the overal deformation of an ensemble of ducts. If this influence is minor, we can rationally forego concerns about characterizing the tribology of molten sodium on metal contact.

6 Path forward, conclusions

At present, this is a modest document intended to frame an opening discussion with our partners having structural mechanics expertise specific to nuclear energy applications. The understanding of requirements and priorities can be codified in a PIRT or similar vehicle. That exercise should include consideration of modeling needs for current and next-gen reactor structural materials. We will refine our list of target validation exercise based upon their further recommendations and understanding of best-available experimental data, and as an alternative, previous analytical studies. A validation study undertaken by early adopters would be mutually beneficial: increasing developer awareness of domain-specific considerations and increasing NE users understanding of Diablo code features, appropriate modeling assumptions and algorithmic trade-offs.

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